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## Sim

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---

### Results of SIM with:

Sequence 1: SEQ (434 residues)  
Sequence 2: [P10845](#), (1296 residues)

### using the parameters:

Comparison matrix: BLOSUM62  
Number of alignments computed: 5  
Gap open penalty: 12  
Gap extension penalty: 4

---



Evaluate the significance of this protein sequence similarity score using [PRSS](#) at [EMBnet-CH](#).

---

99.8% identity in 434 residues overlap; Score: 2296.0; Gap frequency: 0.0%

```
SEQ          1 MSTFTEYIKNIINTSILNLRYESNHLIDLSRYASKINIGSKVNFDPIDKNQIQLFNLESS
P10845,      863 LSTFTEYIKNIINTSILNLRYESNHLIDLSRYASKINIGSKVNFDPIDKNQIQLFNLESS
                *****

SEQ          61 KIEVILKNAIVNSMYENFSTSFWIRIPKYFNSISLNNEYTIINCMENNSGWKVS LNYGE
P10845,      923 KIEVILKNAIVNSMYENFSTSFWIRIPKYFNSISLNNEYTIINCMENNSGWKVS LNYGE
                *****

SEQ          121 IIWTLQDTQEIKQRVVFYKYSQMINISDYINRWIFVTITNNRLNNSKIYINGRLIDQKPIS
P10845,      983 IIWTLQDTQEIKQRVVFYKYSQMINISDYINRWIFVTITNNRLNNSKIYINGRLIDQKPIS
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SEQ          181 NLGNIHASNNIMFKLDGCRDTHRYIWIKYFNLFDKELNEKEIKDLYDNQSN SGILKDFWG
P10845,     1043 NLGNIHASNNIMFKLDGCRDTHRYIWIKYFNLFDKELNEKEIKDLYDNQSN SGILKDFWG
                *****

SEQ          241 DYLYQYDKPYMYMLNLYDPNKYVDVNNVGIRGYMYLKGPRGSVMTTNIYLNSSLYRGTKFII
P10845,     1103 DYLYQYDKPYMYMLNLYDPNKYVDVNNVGIRGYMYLKGPRGSVMTTNIYLNSSLYRGTKFII
                *****
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SEQ 301 KKYASGNKDNIVRNDRVYINVVVKNEYRLATNASQAGVEKILSALEIPDVGNLSQVVV  
P10845, 1163 KKYASGNKDNIVRNDRVYINVVVKNEYRLATNASQAGVEKILSALEIPDVGNLSQVVV  
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SEQ 361 MKSKNDQGITNKCKMNLQDNNGNDIGFIGFHQFNNAKLVASNWNRYQIERSSRTLGCWS  
P10845, 1223 MKSKNDQGITNKCKMNLQDNNGNDIGFIGFHQFNNAKLVASNWNRYQIERSSRTLGCWS  
\*\*\*\*\*

SEQ 421 EFIPVDDGWGERPL  
P10845, 1283 EFIPVDDGWGERPE  
\*\*\*\*\*

---

34.8% identity in 23 residues overlap; Score: 41.0; Gap frequency: 0.0%

SEQ 207 IKYFNLFDKELNEKEIKDLYDNQ  
P10845, 805 VKRLEDFDASLKDALLKYIIDNR  
\* \*\* \*

---

29.4% identity in 34 residues overlap; Score: 39.0; Gap frequency: 0.0%

SEQ 27 IDLSRYASKINIGSKVNFDPIDKNQIQLFNLESS  
P10845, 367 LNFDAVFKINIVPKVNYTIYDGFNLRNTNLAAN  
\*\*\*\* \*\* \*

---

25.0% identity in 28 residues overlap; Score: 39.0; Gap frequency: 0.0%

SEQ 242 YLQYDKPYMYMLNLYDPNKYVDVNNVGIR  
P10845, 366 YLNFDAVFKINIVPKVNYTIYDGFNLR  
\*\* \*\* \*



---

31.8% identity in 22 residues overlap; Score: 37.0; Gap frequency: 0.0%

SEQ 344 LSALEIPDVGNLSQVVVMKSKN  
P10845, 19 IAYIKIPNVGQMGPVKAFKIHN  
\*\* \*\* \*

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Range: from  to 
 Features:
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 ☐ CDD
 ☒ MGC
 ☐ HPRD
 ☐ STS

☐ 1: [P10845](#). Reports Botulinum neuroto...[gi:399133]

[BLink](#), [Links](#)

LOCUS P10845 1296 aa linear BCT 01-MAY-2005  
 DEFINITION Botulinum neurotoxin type A precursor (BoNT/A) (Bontoxilysin A) (BOTOX) [Contains: Botulinum neurotoxin A light-chain; Botulinum neurotoxin A heavy-chain].  
 ACCESSION P10845  
 VERSION P10845 GI:399133  
 DBSOURCE swissprot: locus BXA1\_CLOB0, accession [P10845](#); class: standard.  
 extra accessions: P01561, P18639, created: Jul 1, 1989.  
 sequence updated: Jul 1, 1993.  
 annotation updated: May 1, 2005.  
 xrefs: [X52066.1](#), [CAA36289.1](#), [M30196.1](#), [AAA23262.1](#), [X92973.1](#), [CAA63551.1](#), [D67030.1](#), [BAA11051.1](#), [M27892.1](#), [AAA23269.1](#), [BTCLAB](#), [3BTAA](#)  
 xrefs (non-sequence databases): MEROPSM27.002, InterProIPR008985, InterProIPR011065, InterProIPR006025, InterProIPR000395, PfamPF01742, PRINTSPR00760, ProDomPD001963, PROSITEPS00142  
 KEYWORDS 3D-structure; Direct protein sequencing; Hydrolase; Metalloprotease; Neurotoxin; Pharmaceutical; Protease; Toxin; Transmembrane; Zinc.  
 SOURCE Clostridium botulinum  
 ORGANISM [Clostridium botulinum](#)  
 Bacteria; Firmicutes; Clostridia; Clostridiales; Clostridiaceae; Clostridium.  
 REFERENCE 1 (residues 1 to 1296)  
 AUTHORS Thompson,D.E., Brehm,J.K., Oultram,J.D., Swinfield,T.J., Shone,C.C., Atkinson,T., Melling,J. and Minton,N.P.  
 TITLE The complete amino acid sequence of the Clostridium botulinum type A neurotoxin, deduced by nucleotide sequence analysis of the encoding gene  
 JOURNAL Eur. J. Biochem. 189 (1), 73-81 (1990)  
 PUBMED [2185020](#)  
 REMARK NUCLEOTIDE SEQUENCE.  
 STRAIN=Type A / NCTC 2916  
 REFERENCE 2 (residues 1 to 1296)  
 AUTHORS Binz,T., Kurazono,H., Wille,M., Frevert,J., Wernars,K. and Niemann,H.  
 TITLE The complete sequence of botulinum neurotoxin type A and comparison with other clostridial neurotoxins  
 JOURNAL J. Biol. Chem. 265 (16), 9153-9158 (1990)  
 PUBMED [2160960](#)  
 REMARK NUCLEOTIDE SEQUENCE.  
 STRAIN=Type A / 62A  
 REFERENCE 3 (residues 1 to 1296)  
 AUTHORS East,A.K., Bhandari,M., Stacey,J.M., Campbell,K.D. and Collins,M.D.  
 TITLE Organization and phylogenetic interrelationships of genes encoding

components of the botulinum toxin complex in proteolytic  
Clostridium botulinum types A, B, and F: evidence of chimeric  
sequences in the gene encoding the nontoxic nonhemagglutinin  
component

JOURNAL Int. J. Syst. Bacteriol. 46 (4), 1105-1112 (1996)  
PUBMED [8863443](#)  
REMARK NUCLEOTIDE SEQUENCE OF 1-65.  
STRAIN=Type A / 62A

REFERENCE 4 (residues 1 to 1296)  
AUTHORS Betley,M.J., Somers,E. and DasGupta,B.R.  
TITLE Characterization of botulinum type A neurotoxin gene: delineation  
of the N-terminal encoding region

JOURNAL Biochem. Biophys. Res. Commun. 162 (3), 1388-1395 (1989)  
PUBMED [2669749](#)  
REMARK NUCLEOTIDE SEQUENCE OF 1-34.  
STRAIN=Type A / Hall

REFERENCE 5 (residues 1 to 1296)  
AUTHORS Fujita,R., Fujinaga,Y., Inoue,K., Nakajima,H., Kumon,H. and  
Oguma,K.  
TITLE Molecular characterization of two forms of  
nontoxic-nonhemagglutinin components of Clostridium botulinum type  
A progenitor toxins

JOURNAL FEBS Lett. 376 (1-2), 41-44 (1995)  
PUBMED [8521962](#)  
REMARK NUCLEOTIDE SEQUENCE OF 1-18.  
STRAIN=Type A / NIH

REFERENCE 6 (residues 1 to 1296)  
AUTHORS Schmidt,J.J., Sathyamoorthy,V. and DasGupta,B.R.  
TITLE Partial amino acid sequence of the heavy and light chains of  
botulinum neurotoxin type A

JOURNAL Biochem. Biophys. Res. Commun. 119 (3), 900-904 (1984)  
PUBMED [6370252](#)  
REMARK PROTEIN SEQUENCE OF 1-16.

REFERENCE 7 (residues 1 to 1296)  
AUTHORS Dasgupta,B.R., Foley,J. and Niece,R.  
TITLE Partial sequence of the light chain of botulinum neurotoxin type A

JOURNAL Biochemistry 26, 4162-4162 (1987)  
REMARK PROTEIN SEQUENCE OF 1-46.

REFERENCE 8 (residues 1 to 1296)  
AUTHORS DasGupta,B.R. and Dekleva,M.L.  
TITLE Botulinum neurotoxin type A: sequence of amino acids at the  
N-terminus and around the nicking site

JOURNAL Biochimie 72 (9), 661-664 (1990)  
PUBMED [2126206](#)  
REMARK PROTEIN SEQUENCE OF 1-5 AND 444-456.

REFERENCE 9 (residues 1 to 1296)  
AUTHORS Sathyamoorthy,V., Dasgupta,B.R., Foley,J. and Niece,R.L.  
TITLE Botulinum neurotoxin type A: cleavage of the heavy chain into two  
halves and their partial sequences

JOURNAL Arch. Biochem. Biophys. 266 (1), 142-151 (1988)  
PUBMED [3178218](#)  
REMARK PROTEIN SEQUENCE OF 448-464 AND 872-895.

REFERENCE 10 (residues 1 to 1296)  
AUTHORS Shone,C.C., Hambleton,P. and Melling,J.  
TITLE Inactivation of Clostridium botulinum type A neurotoxin by trypsin  
and purification of two tryptic fragments. Proteolytic action near  
the COOH-terminus of the heavy subunit destroys toxin-binding  
activity

JOURNAL Eur. J. Biochem. 151 (1), 75-82 (1985)  
PUBMED [3896784](#)

REMARK PROTEIN SEQUENCE OF 448-482.  
REFERENCE 11 (residues 1 to 1296)  
AUTHORS Gimenez,J.A. and DasGupta,B.R.  
TITLE Botulinum type A neurotoxin digested with pepsin yields 132, 97, 72, 45, 42, and 18 kD fragments  
JOURNAL J. Protein Chem. 12 (3), 351-363 (1993)  
PUBMED [8397793](#)  
REMARK PROTEIN SEQUENCE OF 866-879 AND 1147-1218.  
REFERENCE 12 (residues 1 to 1296)  
AUTHORS Schiavo,G., Santucci,A., Dasgupta,B.R., Mehta,P.P., Jontes,J., Benfenati,F., Wilson,M.C. and Montecucco,C.  
TITLE Botulinum neurotoxins serotypes A and E cleave SNAP-25 at distinct COOH-terminal peptide bonds  
JOURNAL FEBS Lett. 335 (1), 99-103 (1993)  
PUBMED [8243676](#)  
REMARK IDENTIFICATION OF SUBSTRATE.  
REFERENCE 13 (residues 1 to 1296)  
AUTHORS Binz,T., Blasi,J., Yamasaki,S., Baumeister,A., Link,E., Sudhof,T.C., Jahn,R. and Niemann,H.  
TITLE Proteolysis of SNAP-25 by types E and A botulinum neurotoxins  
JOURNAL J. Biol. Chem. 269 (3), 1617-1620 (1994)  
PUBMED [8294407](#)  
REMARK IDENTIFICATION OF SUBSTRATE.  
REFERENCE 14 (residues 1 to 1296)  
AUTHORS Rigoni,M., Caccin,P., Johnson,E.A., Montecucco,C. and Rossetto,O.  
TITLE Site-directed mutagenesis identifies active-site residues of the light chain of botulinum neurotoxin type A  
JOURNAL Biochem. Biophys. Res. Commun. 288 (5), 1231-1237 (2001)  
PUBMED [11700044](#)  
REMARK MUTAGENESIS OF GLU-261; PHE-265 AND TYR-365.  
REFERENCE 15 (residues 1 to 1296)  
AUTHORS Lacy,D.B., Tepp,W., Cohen,A.C., DasGupta,B.R. and Stevens,R.C.  
TITLE Crystal structure of botulinum neurotoxin type A and implications for toxicity  
JOURNAL Nat. Struct. Biol. 5 (10), 898-902 (1998)  
PUBMED [9783750](#)  
REMARK X-RAY CRYSTALLOGRAPHY (3.3 ANGSTROMS).  
COMMENT On or before Mar 15, 2005 this sequence version replaced [gi:279630](#), [gi:115193](#), [gi:115174](#).  
[FUNCTION] Inhibits acetylcholine release. The botulinum toxin binds with high affinity to peripheral neuronal presynaptic membrane, is then internalized by receptor-mediated endocytosis. The C-terminus of the heavy chain (H) is responsible for the adherence of the toxin to the cell surface while the N-terminus mediates transport of the light chain from the endocytic vesicle to the cytosol. After translocation, the light chain (L) hydrolyzes the 197-Gln-|-Arg-198 bond in SNAP-25, thereby blocking neurotransmitter release. Inhibition of acetylcholine release results in flaccid paralysis, with frequent heart or respiratory failure.  
[CATALYTIC ACTIVITY] Limited hydrolysis of proteins of the neuroexocytosis apparatus, synaptobrevins, SNAP25 or syntaxin. No detected action on small molecule substrates.  
[COFACTOR] Binds 1 zinc ion per subunit.  
[SUBUNIT] Disulfide-linked heterodimer of a light chain (L) and a heavy chain (H).  
[SUBCELLULAR LOCATION] Secreted.  
[PHARMACEUTICAL] Available under the name BOTOX (Allergan) for the treatment of strabismus and blepharospasm associated with dystonia and cervical dystonia. Also used for the treatment of hemifacial

spasm and a number of other neurological disorders characterized by abnormal muscle contraction.

[MISCELLANEOUS] There are seven antigenically distinct forms of botulinum neurotoxin: Types A, B, C1, D, E, F, and G.

[SIMILARITY] Belongs to the peptidase M27 family.

[DATABASE] NAME=BOTOX product information Web site;

WWW='http://www.botox.com/site/'.

[DATABASE] NAME=Protein Spotlight; NOTE=Issue 19 of February 2002;

WWW='http://www.expasy.org/spotlight/back\_issues/sptlt019.shtml'.

FEATURES	Location/Qualifiers
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<u>Region</u>	19..23 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
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	/region_name="Hydrogen bonded turn"
	/evidence=experimental
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	/region_name="Hydrogen bonded turn"
	/evidence=experimental
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<u>Region</u>	600..601
	/gene="botA"
	/region_name="Hydrogen bonded turn"
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Region      618..619
             /gene="botA"
             /region_name="Hydrogen bonded turn"
             /evidence=experimental
Region      622
             /gene="botA"
             /region_name="Beta-strand region"
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Region      625..626
             /gene="botA"
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Region      627..647
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Region      628..629
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             /region_name="Hydrogen bonded turn"
             /evidence=experimental
Region      633
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             /region_name="Beta-strand region"
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             /region_name="Helical region"
             /evidence=experimental
Region      638..644
             /gene="botA"
             /region_name="Hydrogen bonded turn"
             /evidence=experimental
Region      652..659
             /gene="botA"
             /region_name="Helical region"
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Region      656..676
             /gene="botA"
             /region_name="Transmembrane region"
             /note="Potential."
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Region      661..664
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Region      679..681
             /gene="botA"
             /region_name="Beta-strand region"
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Region      688..720
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Region 721
/region_name="Hydrogen bonded turn"
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Region 722..742
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Region 743..745
/region_name="Hydrogen bonded turn"
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Region 746..751
/region_name="Helical region"
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Region 752..753
/region_name="Hydrogen bonded turn"
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Region 758..759
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Region 766..799
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Region 800
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Region 801..824
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Region 825..829
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Region 831..833
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Region 834..835
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Region 836..844
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Region 845..846
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Region 853..855
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Region 860..871
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/gene="botA"
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Region 879..884

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Region 885..886
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Region 887..890
/gene="botA"
/region_name="Beta-strand region"
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Region 891..892
/gene="botA"
/region_name="Hydrogen bonded turn"
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Region 892
/gene="botA"
/region_name="Conflict"
/note="S -> K (in Ref. 8)."
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Region 895..900

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/evidence=experimental
Region 911..912
/gene="botA"
/region_name="Hydrogen bonded turn"
/evidence=experimental
Region 913..917
/gene="botA"
/region_name="Beta-strand region"
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Region 920..921
/gene="botA"
/region_name="Hydrogen bonded turn"
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Region 924..928
/gene="botA"
/region_name="Beta-strand region"
/evidence=experimental
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<u>Region</u>	956..959 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	961..966 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	975..979 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	982..988 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	990..991 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	994..1000 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1011..1012 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1014..1021 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1023..1024 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1026..1031 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1032..1033 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1034..1040 /gene="botA" /region_name="Beta-strand region" /evidence=experimental



<u>Region</u>	1042..1043 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
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<u>Region</u>	1063..1064 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1066..1075 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1081..1090 /gene="botA" /region_name="Helical region" /evidence=experimental
<u>Region</u>	1091..1092 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1094..1095 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1096 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1098 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
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<u>Region</u>	1104 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
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<u>Region</u>	1119..1120 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1122..1125 /gene="botA" /region_name="Beta-strand region" /evidence=experimental

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<u>Region</u>	1152 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1159..1163 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1173 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1175 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1176..1177 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
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<u>Region</u>	1187..1188 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
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<u>Region</u>	1197..1198 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1207..1209 /gene="botA" /region_name="Beta-strand region" /evidence=experimental
<u>Region</u>	1211..1213 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental
<u>Region</u>	1215..1216 /gene="botA" /region_name="Hydrogen bonded turn" /evidence=experimental

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Region      1218
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               /region_name="Beta-strand region"
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Region      1226
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               /region_name="Beta-strand region"
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Region      1228..1229
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               /region_name="Hydrogen bonded turn"
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Region      1232
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Region      1235
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Region      1237..1239
               /gene="botA"
               /region_name="Beta-strand region"
               /evidence=experimental
Region      1242..1243
               /gene="botA"
               /region_name="Hydrogen bonded turn"
               /evidence=experimental
Region      1248..1253
               /gene="botA"
               /region_name="Beta-strand region"
               /evidence=experimental
Region      1260..1264
               /gene="botA"
               /region_name="Beta-strand region"
               /evidence=experimental
Region      1265..1270
               /gene="botA"
               /region_name="Helical region"
               /evidence=experimental
Region      1271..1272
               /gene="botA"
               /region_name="Hydrogen bonded turn"
               /evidence=experimental
Region      1279..1280
               /gene="botA"
               /region_name="Hydrogen bonded turn"

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/gene="botA"  
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Region /evidence=experimental  
1284..1285  
/gene="botA"  
/region\_name="Beta-strand region"  
Region /evidence=experimental  
1289..1290  
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## ORIGIN

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1201 gvekilsale ipdvgnlsqv vvmkskndqg itnkckmnlq dnngndigfi gfhqfnniak
1261 lvasnwynrq ierssrtlgc swefipvddg wgerpl
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